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# Chemical Warfare Agent (CWA) Simulant Project

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**NIOSH/NPPTL Public Meeting  
Hilton Garden Inn, Canonsburg, Pa**

# Purpose of CWA Simulant Project

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Stakeholder wanted NIOSH to Identify chemical compounds that can simulate the permeation effects of GB and HD

# Project Goals (Phase I)

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- Identify chemical compounds that simulate the permeation effect of GB and HD through barrier materials
- Develop a laboratory procedure that can be used by stakeholders for estimating permeation breakthrough times using (GB and HD) simulants
- Provide Stakeholders with a low cost, rapid screening method for evaluating materials using available, low toxic simulants

# Accomplishments (Phase I)

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- 1.) Based on correlation, identified four (4) simulants that can be used to estimate CWA permeation through barrier materials:
  - Nominal HD simulants
    - DCH - 1,6-Dichlorohexane
    - CEPS - 2-Chloroethyl phenyl sulfide
  - Nominal GB simulants
    - DEMP - Diethyl methylphosphonate
    - DIMP - Diisopropyl methylphosphonate

# Accomplishments (Phase I)

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## 2.) Developed test procedure

- Used for testing liquid permeation resistance through nonporous barrier polymers
- Uses a new cell design, the Flooded Cell Technique, for testing both hard and soft barrier materials up to 1.0 cm thick
- Flooded Cell Technique: challenging chemical compound covers the entire surface area of the test specimen

# Accomplishments (Phase I)

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## 3.) Developed written test method

- Describes required equipment, procedures, and data analysis techniques; Also, includes mechanical drawings of permeation cell
- Test method will be published as an official NIOSH numbered document
- Status of document: peer review process initiated which will include (verification testing) of test method

# Project Goals (Phase II)

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- Improve estimation reliability of Flooded Cell Technique by testing additional simulants with other barrier materials
- Determine quantitative relationship between Flooded Cell Technique and conventional test loading ( $10 \text{ g/m}^2$ )
- Determine CWA/simulant sorption/desorption of representative barrier materials

# Project Goals (Phase II) (cont)

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- Identify critical properties of permeants and barrier materials that control permeation
- Develop capability to predict barrier permeation based on available chemical and physical properties of barrier polymers and permeating molecule



# Project Status (Phase II)

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## Candidate materials selected

- **Thermoplastics:**
  - PVDF [Poly(vinylidene fluoride)] 0.05 mm
  - PP [Polypropylene] 0.04 mm
  - PET [Poly(ethylene terephthalate)] 0.006 mm
- **Elastomers:**
  - Poly(tetrafluoroethylene-co-propylene)  
AFLAS<sup>TM</sup> rubber 0.8–2.4mm

# Project Status (Phase II) (cont)

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## Comparison tests

- Flooded cell vs. conventional (10 gm/m<sup>2</sup>) w/DIMP and DCH on butyl
- Breakthrough times essentially equal

# Summary/Conclusion

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- Developed a rapid, relatively low cost laboratory procedure that can be used to estimate CWA permeation through barrier materials
- Identified four (4) CWA simulants for permeation testing
- Developed written test method that describes equipment, test procedures, and data analysis techniques: peer review process initiated

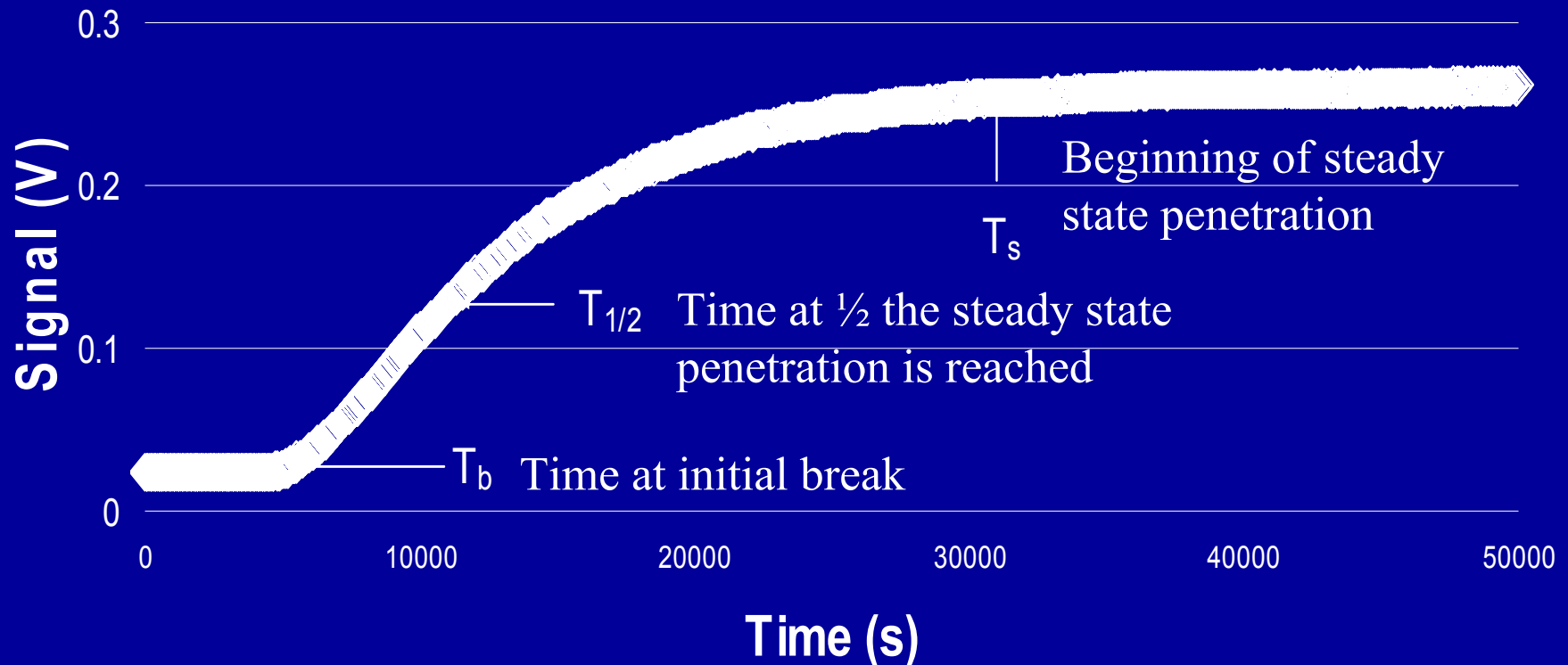
# Summary/Conclusion (cont)

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- Initiated Phase II of the CWA Simulant Project

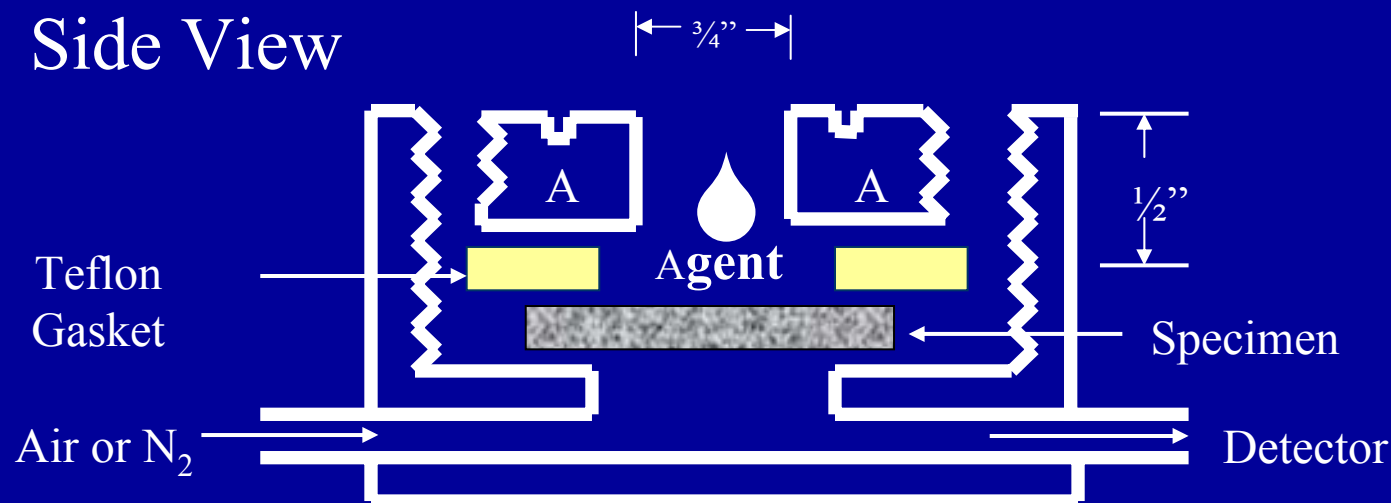
**Note: NIOSH or RDECOM does not guarantee that simulants identified will be suitable for all materials, nor does passage of manufacturer's pretest with a simulant guarantee passage of the official NIOSH certification testing**

# Liquid Permeation of EPDM with DIMP

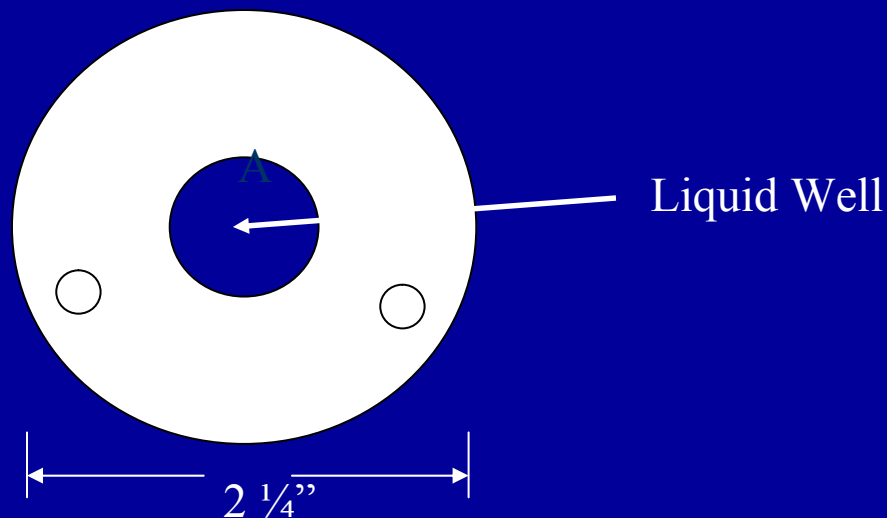


# Liquid Permeation Cell Component

Side View



Top View



# Permeation Cell Photographs

